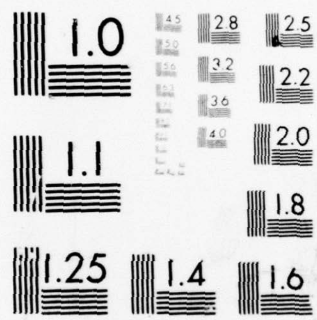
AD-A069 788 CATHOLIC UNIV OF AMERICA WASHINGTON D C F/G 20/8
ELECTRONIC STOPPING POWER CALCULATIONS.(U)
JUN 79 J G BRENNAN, D J LAND N00014-78-C-0515
UNCLASSIFIED NL

| OF |
AD
A069788

END
DATE
FILMED
7 -- 79
DDC



MICROCOPY RESOLUTION TEST CHART
NATIONAL BUREAU OF STANDARDS-1963-A

UNCLASSIFIED

SECURITY CLASSIFICATION OF THIS PAGE (When Data Entered)

AD A069788

DDC FILE COPY

12

REPORT DOCUMENTATION PAGE

READ INSTRUCTIONS BEFORE COMPLETING FORM

1. REPORT NUMBER
#1

2. GOVT ACCESSION NO.

3. RECIPIENT'S CATALOG NUMBER

4. TITLE (and Subtitle)
6 ELECTRONIC STOPPING POWER CALCULATIONS

5. TYPE OF REPORT & PERIOD COVERED
Annual Summary June [redacted] 78- [redacted] May [redacted] 979

6. PERFORMING ORG. REPORT NUMBER

LEVEL

7. AUTHOR(s)
10 J. G. Brennan
D. J. Land

8. CONTRACT OR GRANT NUMBER(s)
15 N00014-78-C-0515 new

9. PERFORMING ORGANIZATION NAME AND ADDRESS
The Catholic University of America
Washington, D.C. 20064

10. PROGRAM ELEMENT, PROJECT, TASK AREA & WORK UNIT NUMBERS
NR 020-038/5/11/78 (421)

11. CONTROLLING OFFICE NAME AND ADDRESS
Office of Naval Research, Director, Physics Progr.
Physical Sciences Division
800 N. Quincy St., Arlington, Va. 22217

12. REPORT DATE
11 4 June [redacted] 979

13. NUMBER OF PAGES
4

14. MONITORING AGENCY NAME & ADDRESS (if different from Controlling Office)
Office of Naval Research, Director, Physics Progr.
Physical Sciences Division
800 N.Quincy St.,Arlington, Va. 22217

15. SECURITY CLASS. (of this report)
unclassified

15a. DECLASSIFICATION/DOWNGRADING SCHEDULE

16. DISTRIBUTION STATEMENT (of this Report)

Approved for public release; distribution unlimited

9 Annual summary rept. no. 1,
1 Jun 78-31 May 79,

DDC

RECEIVED JUN 12 1979

C

17. DISTRIBUTION STATEMENT (of the abstract entered in Block 20, if different from Report)

NA 12 5p.

18. SUPPLEMENTARY NOTES

NA

19. KEY WORDS (Continue on reverse side if necessary and identify by block number)

Stopping Powers, Ion Implantation

076 400 Gw

20. ABSTRACT (Continue on reverse side if necessary and identify by block number)

The electronic stopping power values for projectiles whose atomic number lies between 6 and 92, incident on targets from Z = 1 to Z = 102 has been calculated using Hartree-Fock wave functions within the Firsov context. Relativistic corrections have been included. Comparisons of these stopping power values with all existing experimental values are made. Part of this work has been published and the rest will be published as a technical report. An outline of proposed study for the coming year is presented.

DD FORM 1 JAN 73 1473 EDITION OF 1 NOV 65 IS OBSOLETE
S/N 0102-LF-014-6601

UNCLASSIFED

SECURITY CLASSIFICATION OF THIS PAGE (When Data Entered)

ELECTRONIC STOPPING POWER CALCULATIONS

ANNUAL SUMMARY

This report is a summary of work completed during the first year of the contract, June 1, 1978 to May 31, 1979. It is a joint effort between Dr. J. G. Brennan of The Catholic University of America and Dr. D. J. Land of the Naval Surface Weapon Center.

The purpose of this theoretical study is to calculate more precise values for the electronic stopping powers of low velocity heavy ions ($v \leq v_0 = \varepsilon^2/\hbar$). The method has been described in the Office of Naval Research proposal and in several publications of the coworkers. The effort this year has been directed toward completing the Z_1, Z_2 matrix of stopping power values to include projectiles and targets for all Z greater than 54. This calculation has been accomplished and will be issued as a technical report at the end of the summer. The matrix of stopping powers for Z less than 54 has recently been published in "Atomic and Nuclear Data Tables".

The most important issue which will be discussed in the technical report is to compare these theoretical stopping power values for high Z projectiles and targets with experiments. This is not easy to do because the experimental results for low-velocity projectiles are sparse. Most projectiles between Z=6 and Z=20 have been used on targets of carbon, aluminum, nickel, silver, and gold. Also, carbon, nitrogen, oxygen, and neon projectiles have been studied on a variety of gaseous targets, primarily the noble gases. Bromine, chlorine, iodine, and uranium projectiles have also been studied as they traversed carbon, aluminum, nickel, silver, and gold. Finally there is an extensive set of data for lithium and nitrogen projectiles incident on targets from Z=6 to Z=52. There are some other isolated measurements of stopping powers but at velocities too high to be of use for our calculations.

In a previous article, the authors discussed a procedure for extrapolating electronic stopping powers to velocities above v_0. What we suggested was a straight line fit from our calculated values valid at v_0 to the values at a velocity where the scaling law commenced to be valid. We found that if we choose this point at a velocity of $2v_0$, we obtained reasonably good agreement with those experimental data available except for the heaviest projectile, uranium. For this case we found that a value at $3v_0$ gave better agreement.

Recently we have investigated this question and now feel that it can be understood at least qualitatively by the determination of how many "outer electrons" a projectile must shed before the scaling laws become operable. By outer electrons, we mean in this context, those electrons which give significant contributions to the electronic stopping within the Firsov framework. In other words, we are defining outer electrons of a projectile as those which give the observed structure to the electronic stopping power values as calculated at v_0. Once these electrons have been stripped from the projectile, the ion behaves as a structureless particle and the scaling law can be used. We have determined the number of outer electrons for all projectiles on this basis. It is not surprising to find that for those projectiles with Z above 20 for which data exist, namely the halogens and uranium, uranium has twice as many outer electrons as do the halogens. Thus it seems clear why the scaling law does not become operable for uranium until a higher velocity is reached than for the other projectiles. Our calculations indicate that many other projectiles have large numbers of outer electrons but, unfortunately, no experimental data exist for these cases.

The stopping power calculations employed relativistic Hartree-Fock wave functions for Z_2 greater than 54. For comparison, a group of targets in this region were calculated using nonrelativistic Hermann Skillman wave

functions. Although individual atomic shell contributions might differ in the two cases by as much as 20%, the relativistic and nonrelativistic wave functions gave results for the total stopping which differed by less than 5%. Because of this insensitivity, the stopping powers of the heavy projectiles, Z_1 greater than 54 were calculated using the Hermann Skillman nonrelativistic wave functions. It was felt that this part of the matrix is somewhat less useful in practice and did not justify the use of relativistic ionic wave functions which would require more computor time. However, a brief study on this point is in order in the coming year in view of the 20% individual shell differences found for the targets.

As we will detail in our technical report, the values of electronic stopping which we have calculated for this matrix give good correlation with existing experimental data. However, these calculations which are based on a model originated by Firsov are not susceptible of explaining certain features of the data. The Firsov model essentially leads to complete symmetry between Z_1 and Z_2 oscillations. However, a close scrutiny of the data reveal small but important differences. For example, the variationsof S_e as a function of Z_2 rises quite steeply from minima at the noble gases to maxima, whereas the variation with Z_1 indicates a more gradual rise of the stopping powers.

There is another method of calculating stopping powers due to Lindhard. The Lindhard model, which is based upon the coulomb interactions between projectile and target is more physically motivated than is the Firsov model which is based on the mechanical transfer of electrons. We chose the Firsov model originally because it was possible to modify it to put in more realistic atomic wave functions for both projectile and target. Recently Ritchie of Oak Ridge has made some progress in modifying the Lindhard model to contain details of the projectile system, but so far for only the lightest projectiles. We shall be seeking to extend these modifications to other

projectiles. Such an approach may succeed in explaining the observed lack of symmetry in Z_1 and Z_2 as discussed above. The Lindhard Model may also provide a method to include the difference between solid and gaseous targets. We shall also attempt to study the charge state behavior of the projectiles as a function of increasing velocity. Our previous attempts to account for nonlinear behavior of S_e with velocity within the Firsov framework were not successful. The extension of the Lindhard model will therefore be an important goal of the next year's activities.

The cooperation between Dr. Brennan of Catholic University and Dr. Land of the Naval Surface Weapons Center continued throughout the year. Dr. Brennan spent the Summer of 1978 and the Spring and Summer of 1979 at NSWC. Dr. Brennan and Dr. Land visited the Oak Ridge National Laboratory and Dr. Brennan also visited atomic physics groups at Kansas State University, the University of Arizona, and Stanford University.